Superconductivity with hard-core repulsion: BCS-Bose crossover and s-/d-wave competition

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We consider fermions on a 2D lattice interacting repulsively on the same site and attractively on the nearest neighbor sites. The model is relevant, for instance, to study the competition between antiferromagnetism and superconductivity in a Kondo lattice. We first solve the two-body problem to show that in the dilute and strong coupling limit the s-wave Bose condensed state is always the ground state. We then consider the many-body problem and treat it at mean-field level by solving exactly the usual gap equation. This guarantees that the superconducting wave-function correctly vanishes when the two fermions (with antiparallel spin) sit on the same site. This fact has important consequences on the superconducting state that are somewhat unusual. In particular this implies a radial node-line for the gap function. When a next neighbor hopping t' is present we find that the s-wave state may develop nodes on the Fermi surface.

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I. INTRODUCTION

Superconductivity is possible when carriers attract. The attraction in metals is normally due to the phonon coupling. The strong coulomb repulsion is normally well screened in metals and under some conditions it can be overcome by the attraction leading to superconductivity. A locally attractive (non-retarded) model, such as the BCS one, can thus give a good qualitative description of the superconducting state since the correlation length ξ is much larger than both the screening length and the interparticle density.

This is not the case when the carriers are non conventional. A relevant example is the single-band Kondo lattice with a RKKY interaction. For large Kondo coupling the ground state of this system is formed by local singlets: it is thus insulating at half-filling. At small doping the carriers are bachelor spins: they feel a hard core repulsion, since they cannot sit on the same site at the same time. The RKKY antiferromagnetic exchange interaction gives an attraction among holes in the singlet channel, and thus it could lead to a superconducting state^{1,2}. But in this case the hard-core repulsion cannot be neglected in the description of the s-wave superconductivity. More details on the Kondo lattice model are discussed in Reference 2.

In this paper we consider a simple model where the role of the hard-core repulsion can be analyzed in a transparent way. For simplicity and relevance to physical systems we consider a two dimensional square lattice with hopping and attractive interaction among nearest neighbor sites. Different range for the interaction and the hopping produces interesting results, that will be ana-

lyzed. Similar models have been studied by different authors. Ohkawa and Fukuyama proposed an ansatz to solve the mean-field equations for superconductivity with local repulsion in Kondo systems³. Later Micnas, Ranninger, and Robaszkiewicz⁴ and Bastide, Lacroix, and Rosa Simoes⁵, applied that technique to calculate the superconducting critical temperature. Similar equations in a different context were considered by Aligia and coworkers.⁶

We will reconsider the problem at zero temperature and investigate the competition among different symmetries of the order parameter as one spans the crossover from BCS superconductivity to Bose condensation^{7,8,9,10,11,12,13,14,15,16}. In particular we will clarify an apparent disagreement with the prediction of Randeria¹⁷ on the presence of bound states and superconducting instabilities in 2D systems. We will also discuss the unusual nature of the superconducting state: the main peculiarity is the presence of a radial line of nodes in k space for the gap function $\Delta(\mathbf{k})$.

The plan of the paper is the following. In Section II we define in detail the model we are considering. In Section III we solve the two body problem and we discuss the relevance to the Bose limit. In Section IV we set up the mean field equations and find the resulting phase diagram for the ground state. The competition between s- and d-wave superconductivity is analyzed in Section V. In Section VI the effect of a mismatch between the hopping and the interaction range is considered by introducing a hopping t' among next-neighbor sites.

II. THE MODEL

We consider fermions hopping on a 2D square lattice of spacing a with nearest-neighbor sites hopping matrix elements t. (In some cases we will consider also next-neighbor hopping t'.) The fermions interact with a local repulsive interaction parameterized by U, that we will set to infinity. They furthermore feel an attraction V, which we assume to act only between nearest neighbors (in a real RKKY example that would not be the case) with opposite spins. The relevant parameters at zero temperature are only V/t and the filling of the band 0 < n < 2. The spin does not play an essential role. Since we are interested in the singlet state, we can disregard the parallel-spin part of the interaction, the mean field equations would not be modified by that. The model Hamiltonian is thus:

$$H = \sum_{\mathbf{k}\sigma} (t_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + U \sum_{i} (n_{i\uparrow} - \frac{1}{2}) (n_{i\downarrow} - \frac{1}{2})$$
$$-V \sum_{i,\delta} (n_{i\uparrow} - \frac{1}{2}) (n_{i+\delta\downarrow} - \frac{1}{2})$$
(1)

where the vector δ spans the four nearest neighbor sites of the square lattice, σ is the spin projection in a chosen direction and $t_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a)]$ is the single-particle dispersion relation.

The Hamiltonian in the form of Eq. (1) is particle-hole symmetric: for half-filling $\mu = 0$. For convenience it can also be written in a non p-h symmetric, but shorter form:

$$H = \sum_{\mathbf{k}\sigma} (t_{\mathbf{k}} - \mu_o) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - V \sum_{i,\delta} n_{i\uparrow} n_{i+\delta\downarrow} ,$$
(2)

where $\mu_o = \mu + (U - 4V)/2$. The two forms are equivalent but from a constant. The interaction term can be written in Fourier space as usual:

$$\sum_{\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4} V(\mathbf{k}_2 - \mathbf{k}_3) c_{\mathbf{k}_1 \uparrow}^{\dagger} c_{\mathbf{k}_2 \downarrow}^{\dagger} c_{\mathbf{k}_3 \downarrow} c_{\mathbf{k}_4 \uparrow}$$
(3)

with $V(\mathbf{k}) = U - Vw(\mathbf{k})$ and $w(\mathbf{k}) = \sum_{\delta} e^{i\mathbf{k}\delta} = 2[\cos(k_x a) + \cos(k_y a)].$

In the following we investigate the superconducting order in the ground state of the Hamiltonian (1). In order to treat the strong repulsion correctly we consider first the two body problem, that is relevant in the dilute limit.

III. TWO-BODY PROBLEM

If the attractive interaction is strong enough to bind a pair we expect to reach the Bose condensed limit for a low density of carriers. It is thus crucial to know whether a bound state is present or not. In our case the hard-core repulsion will fight against an s-wave bound state, while it will not affect the d-wave state. In the dilute limit the

choice between s- and d-wave is determined simply by the lowest 2-body bound state, if present.

We thus begin our investigation by solving the two body problem: we find the threshold for the appearance of bound states. The two-body problem is exactly solvable by diagonalization of a 5 by 5 matrix, corresponding to the central and 4 neighbor sites involved in the equations of motions. This can be done directly in real space, but we will proceed in momentum space in order to use the same approach for the mean field equations in the next Section. In k-space the simplification comes from the separability of the interaction potential. As a matter of fact, $V_{\mathbf{k}\mathbf{k}'} = V(\mathbf{k} - \mathbf{k}')$, defined above can be written in a separable form as follows:

$$V_{\mathbf{k}\mathbf{k}'} = \sum_{\alpha\beta} w_{\alpha}(\mathbf{k}) \, \mathcal{V}_{\alpha\beta} \, w_{\beta}(\mathbf{k}') \tag{4}$$

where

$$\begin{cases}
w_0(\mathbf{k}) = 1 \\
w_1(\mathbf{k}) = [\cos(k_x a) + \cos(k_y a)]/\sqrt{2} \\
w_2(\mathbf{k}) = [\cos(k_x a) - \cos(k_y a)]/\sqrt{2} \\
w_3(\mathbf{k}) = \sin(k_x a) \\
w_4(\mathbf{k}) = \sin(k_y a)
\end{cases} (5)$$

 $V_{\alpha\beta} = v_{\alpha}\delta_{\alpha\beta}$, with $v_0 = U$ and $v_{\alpha} = -2V$ for $\alpha \neq 0$. We have chosen a symmetrized and anti-symmetrized combination of cosines in order to exploit the symmetry of the lattice.

The Green's function for the two-body problem on the basis $|\mathbf{q}\mathbf{Q}\rangle=c_{\mathbf{q}+\mathbf{Q}/2\uparrow}^{\dagger}c_{-\mathbf{q}+\mathbf{Q}/2\downarrow}^{\dagger}|0\rangle$ is diagonal in \mathbf{Q} . We consider only the case $\mathbf{Q}=0^{18}$. The corresponding equation of motion is thus that of a particle in an external potential:

$$(\omega - 2t_{\mathbf{k}})\mathcal{G}_{\mathbf{k}\mathbf{p}}(\omega) - \sum_{\mathbf{q}} V_{\mathbf{k},\mathbf{q}}\mathcal{G}_{\mathbf{q}\mathbf{p}}(\omega) = \delta_{\mathbf{k}\mathbf{p}}.$$
 (6)

Since V is separable the above integral equation reduces to an algebraic one for 5 parameters. The substitution of the separable form of V gives:

$$(\omega - 2t_{\mathbf{k}})\mathcal{G}_{\mathbf{k}\mathbf{p}}(\omega) - \sum_{\alpha} w_{\alpha}(\mathbf{k})A_{\alpha\mathbf{p}}(\omega) = \delta_{\mathbf{k}\mathbf{p}}, \quad (7)$$

where

$$A_{\alpha \mathbf{p}}(\omega) = v_{\alpha} \sum_{\mathbf{q}} w_{\alpha}(\mathbf{q}) \mathcal{G}_{\mathbf{q}\mathbf{p}}(\omega).$$
 (8)

The Green's function is thus:

$$\mathcal{G}_{\mathbf{k}\mathbf{p}}(\omega) = \mathcal{G}_{\mathbf{k}}^{o}(\omega) \left[\delta_{\mathbf{k}\mathbf{p}} + \sum_{\alpha} w_{\alpha}(\mathbf{k}) A_{\alpha\mathbf{p}}(\omega) \right], \quad (9)$$

where $\mathcal{G}_{\mathbf{k}}^{o}(\omega) = (\omega - 2t_{\mathbf{k}})^{-1}$. Substituting (9) into (8) we obtain the following closure equation for $A_{\alpha \mathbf{p}}$:

$$A_{\alpha \mathbf{p}}(\omega) = v_{\alpha} w_{\alpha}(\mathbf{p}) \mathcal{G}_{\mathbf{p}}^{o}(\omega) + v_{\alpha} \sum_{\beta} B_{\alpha \beta}(\omega) A_{\beta \mathbf{p}}(\omega) , \quad (10)$$

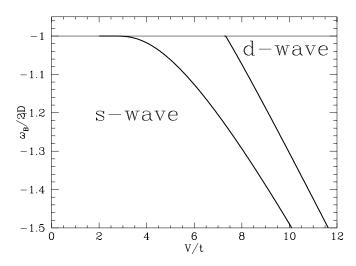


FIG. 1: Two-body s-wave and d-wave bound state energy as a function of V/t and measured in terms of the band width 2D=8t. In both cases we find a threshold for the appearance of the bound state.

where

$$B_{\alpha\beta}(\omega) = \sum_{\mathbf{q}} w_{\alpha}(\mathbf{q}) w_{\beta}(\mathbf{q}) \mathcal{G}_{\mathbf{q}}^{o}(\omega).$$
 (11)

The set of linear equations (10) for A can be solved by inversion of the 5x5 matrix, $1 - \mathcal{V} B(\omega)$

$$A_{\alpha \mathbf{p}}(\omega) = \sum_{\beta} \mathcal{T}_{\alpha \beta}(\omega) w_{\beta}(\mathbf{p}) \mathcal{G}_{\mathbf{p}}^{o}(\omega)$$
 (12)

where we have defined $\mathcal{T}(\omega) = [1 - \mathcal{V}B(\omega)]^{-1}\mathcal{V}$. The final expression for the Green's function is:

$$\mathcal{G}_{\mathbf{k}\mathbf{p}}(\omega) = \mathcal{G}_{\mathbf{k}}^{o}(\omega) \left[\delta_{\mathbf{k}\mathbf{p}} + \mathcal{G}_{\mathbf{p}}^{o}(\omega) \sum_{\alpha\beta} \mathcal{T}_{\alpha\beta}(\omega) w_{\alpha}(\mathbf{k}) w_{\beta}(\mathbf{p}) \right].$$
(13)

Note that \mathcal{T} is the usual T-matrix of scattering theory:

$$T_{\mathbf{k}\mathbf{p}} = \sum_{\alpha\beta} \mathcal{T}_{\alpha\beta} w_{\alpha}(\mathbf{k}) w_{\beta}(\mathbf{p}). \tag{14}$$

The problem can now be solved for any value of U, but since we are interested in the $U=\infty$ limit it is convenient to write \mathcal{T} as:

$$\mathcal{T} = (\mathcal{V}^{-1} - B)^{-1} \tag{15}$$

where $(\mathcal{V}^{-1})_{00} = 1/U = 0$. In this way we eliminate U from the outset. One can readily verify that for $U = \infty$ the resulting local Green function $\mathcal{G}(\mathbf{x}_i = 0)$ actually vanishes. As it should, the hard-core repulsion prevents two fermions with opposite spin projection to sit on the same site.

Let us come back to the explicit evaluation of \mathcal{T} in two dimensions. The B matrix is in block form, $\mathcal{G}^o_{\mathbf{q}}$ is in fact even under both $k_x \to -k_x$ and $k_y \to -k_y$. w_2 is odd under $k_x \leftrightarrow k_y$, and w_3 and w_4 are odd under $k_x \to -k_x$ and $k_y \to -k_y$ respectively. These symmetries leave few non vanishing elements and split the matrix in block form, corresponding to the irreducible representations of the symmetry group of the lattice:

$$B = \begin{pmatrix} B_{00} & B_{01} & 0 & 0 & 0 \\ B_{01} & B_{11} & 0 & 0 & 0 \\ 0 & 0 & B_{22} & 0 & 0 \\ 0 & 0 & 0 & B_{33} & 0 \\ 0 & 0 & 0 & 0 & B_{33} \end{pmatrix} . \tag{16}$$

The bound states are given by the solution of the equation $\det(\mathcal{V}^{-1} - B) = 0$. We obtain thus the following equations:

$$\frac{1}{2V} = \frac{B_{01}^2}{B_{00}} - B_{11} \,, \tag{17}$$

$$-\frac{1}{2V} = B_{22} = \frac{1}{2} \sum_{\mathbf{k}} \frac{[\cos(k_x a) - \cos(k_y a)]^2}{\omega - 2t_{\mathbf{k}}}, (18)$$

$$-\frac{1}{2V} = B_{33} = \sum_{\mathbf{k}} \frac{\sin^2(k_x a)}{\omega - 2t_{\mathbf{k}}}.$$
 (19)

Eqs. (17), (18), and (19) refer to s-, d-, and p-wave bound states, respectively. An additional s-wave bound state has been eliminated by setting $U=\infty$. Note that U does not affect the p- and d-solutions, since the wavefunction vanishes at the origin. In contrast, the s-wave bound state is strongly affected by U. As a matter of fact, $B_{00}(\omega)$, $B_{01}(\omega)$, and $B_{11}(\omega)$ all diverge logarithmically for $\omega \to 2D = 8t$, with 2D the single particle band width. Using Eqs. (20) and (21) below one can verify that these divergences disappears in Eq. (17), due to mutual cancellation: the s-wave bound state is present only for V larger than a threshold V_t^s , while for a purely attractive potential binding always occurs in two-dimensions.

It is not difficult to prove the following exact relations among the different B's by summing and subtracting ω and cosine terms in the numerator:

$$\omega B_{00}(\omega) + 4\sqrt{2} t B_{01}(\omega) = 1, \qquad (20)$$

$$\omega B_{01}(\omega) + 4\sqrt{2}tB_{11}(\omega) = 0. \tag{21}$$

Substituting Eqs. (20) and (21) into Eq. (17) the s-wave bound state equation becomes:

$$\frac{2t}{V} = -\frac{\omega}{8t} + \frac{1}{8t B_{00}(\omega_B)} \qquad s-\text{wave}, \qquad (22)$$

where explicitly $B_{00}(\omega) = \sum_{\mathbf{k}} (\omega - 2t_{\mathbf{k}})^{-1}$. At the threshold V_t^s the bound state energy lies at the band bottom $\omega = -8t$ where B_{00} diverges: hence the threshold V_t^s for a s-wave bound state is simply V = 2t. The s-wave solution appears non analytically at the threshold: $\omega_B(V) \approx -2D - 4t \exp\{-\pi V_t^s/(V - V_t^s)\}$. For values

of $V > V_t^s$ Eq. (22) can be solved numerically. We plot the result in Figure 1 together with the d-wave bound state energy obtained by numerical solution of Eq. (18). As it can be seen from the picture the d-wave threshold $V_c^d \approx 7.35\,t$ is higher than the s-wave one, (despite the fact that the latter is affected by the hardcore). This reflects the cost in kinetic energy (curvature of the wave functions) of changing the sign as we go around $\mathbf{x}=0$.

We thus conclude that for $V > V_t^s$ and for low density the ground state of the system is a Bose condensate of fermions pairs in a s-wave bound state. The Bose limit is safely achieved only if the bound state energy, $|\omega_B + 2D|$, is much larger than the interparticle distance energy scale, i.e. $\epsilon_F \sim t\,n$. Since $\omega_B + 2D$ vanishes exponentially near V_c the Bose region in the n-V diagram rapidly shrinks as $V \to V_c$ (cf. Fig. 2 in the following).

This picture for dilute pairs is quite clear and it will not be modified by the introduction of a small t' (see following discussion). The opposite BCS limit is on the other hand more subtle.

IV. MEAN FIELD EQUATIONS FOR SUPERCONDUCTIVITY

In order to study the onset of superconductivity for small coupling and large density, we consider the usual BCS mean field theory.

As in the two-body problem, the integral equation can be reduced to a simple algebraic equation. The s-wave solution is strongly modified by the hard-core interaction, and the order parameter has a \mathbf{k} dependence that comes from the mixing of the w_0 and w_1 terms, as in the two body problem. This mixing is crucial in order to ensure the vanishing of the superconducting wavefunction at the origin.

The mean-field theory equations describing the superconducting state of the Hamiltonian (1) are obtained by the usual decoupling:

$$H_{MF} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{k} \left[\Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} + cc \right] . \quad (23)$$

The minimization procedure gives the familiar equations for the ground state:

$$n = \sum_{\mathbf{k}} \left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right], \tag{24}$$

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V(\mathbf{k} - \mathbf{k}') \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}, \qquad (25)$$

where $\xi_{\mathbf{k}} = t_{\mathbf{k}} - \mu_o + V(0)n/2$, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$, and for consistency we retained the Hartree term. Putting together the Hartree shift and the original shift of the chemical potential we have $\xi_{\mathbf{k}} = t_{\mathbf{k}} - \mu'$, with $\mu' = \mu + \frac{1}{2}(U - 4V)(n - 1)$. (There is no Fock exchange term because of our interaction between opposite spins only.)

We concentrate now on the gap equation (25). We exploit again the separability of the interaction to write:

$$\Delta_{\mathbf{k}} = -\sum_{\alpha} v_{\alpha} w_{\alpha}(\mathbf{k}) \sum_{\mathbf{k}'} w_{\alpha}(\mathbf{k}') \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} = \sum_{\alpha} A_{\alpha} w_{\alpha}(\mathbf{k}),$$
(26)

where the new coefficients A satisfy:

$$A_{\alpha} = -v_{\alpha} \sum_{\beta} W_{\alpha\beta}[A] A_{\beta} , \qquad (27)$$

and we have defined the matrix W, analogous of the matrix B for the two-body problem:

$$W_{\alpha\beta}[A] = \sum_{\mathbf{k}} \frac{w_{\alpha}(\mathbf{k})w_{\beta}(\mathbf{k})}{2E_{\mathbf{k}}}.$$
 (28)

The A dependence comes through Δ in E. In matrix form Eq. (27) reads simply $(1 + \mathcal{V}W)A = 0$. As before it is convenient to write the equation for A in terms of \mathcal{V}^{-1} , in order to perform easily the limit $U \to \infty$. Eq. (27) thus becomes:

$$(\mathcal{V}^{-1} + W[A])A = 0. (29)$$

In order to find $\Delta_{\mathbf{k}}$ we need to solve the nonlinear equation (29), analogous of the linear equation (10) for the two-body problem. Let λ_i and v_{α}^i be the eigenvalues and eigenvectors of $\mathcal{V}^{-1} + W$. We project $A_{\alpha} = \sum_i c_i v_{\alpha}^i$ on the v_{α}^i , so that

$$\sum_{i} \lambda_i[c]c_i v^i = 0 \tag{30}$$

 c_i is non vanishing only if $\lambda_i = 0$. The corresponding coefficient $c = c_i$ is fixed by the equation $\lambda_i[c] = 0$. The form of the solution for A is simply $A_{\alpha} = cv_{\alpha}^i$, and for $\Delta_{\mathbf{k}} = c\sum_{\alpha} v_{\alpha}^i w_{\alpha}(\mathbf{k})$.

Due to the symmetry of the crystal, the matrix W is already in the form (30) for $\alpha = 2$, 3, and 4. The conditions $\lambda_i = 0$ in these cases give the two equations

$$\frac{1}{2V} = \frac{1}{2} \sum_{\mathbf{k}} \frac{[\cos(k_x a) - \cos(k_y a)]^2}{2E_{\mathbf{k}}}, \quad (31)$$

$$\frac{1}{2V} = \sum_{\mathbf{k}} \frac{\sin^2(k_x a)}{2E_{\mathbf{k}}},\tag{32}$$

that correspond to the d- and p-wave solutions. In the "s" subspace $\{w_0, w_1\}$ we are instead left with a 2 by 2 matrix:

$$\mathcal{V}^{-1} + W[A] = \begin{pmatrix} W_{00} & W_{01} \\ W_{01} & -1/2V + W_{11} \end{pmatrix}. \tag{33}$$

The condition of vanishing of the determinant gives:

$$-\frac{1}{2V} = \frac{W_{01}^2}{W_{00}} - W_{11} \,, \tag{34}$$

When a solution is found the form of the gap function will be given by the corresponding eigenvector of (33): $v = (W_{01}, -W_{00})$, thus

$$\Delta_{\mathbf{k}} = \Delta \left[1 - r \frac{\cos k_x a + \cos k_y a}{\sqrt{2}} \right] \tag{35}$$

where

$$r = W_{00}/W_{10} \,. \tag{36}$$

The mixing of the two w's is crucial in order to take into account correctly the hard-core repulsion. This was already clear from the two-body problem, where the exact solution gives a wave function that is a superposition of w_0 and w_1 . At the MF level we could, in principle, search for solutions with only one of these two components different from zero: such a procedure is wrong. The simplest way to see that is to evaluate the anomalous correlation function $\mathcal{F}(\mathbf{x}-\mathbf{y}) = \langle c_{\uparrow}(\mathbf{x})c_{\downarrow}(\mathbf{y})\rangle$. This function is the equivalent of the wavefunction for the two-body problem: it gives the probability of finding two fermions on the same site, thus for infinite U it is bound to be zero at the origin. We can verify that our solution correctly gives $\mathcal{F}(0) = 0$:

$$\mathcal{F}(0) = \sum_{\mathbf{k}} \mathcal{F}_{\mathbf{k}} = \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

$$\propto \left[W_{01} \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}} - W_{00} \sum_{\mathbf{k}} \frac{w_1(\mathbf{k})}{E_{\mathbf{k}}} \right] = 0 \qquad (37)$$

It is clear that if, out of the two order parameters, only one is present, $\mathcal{F}(0)$ would be always non-vanishing. For p- and d-wave, the symmetry alone is sufficient to guarantee the vanishing of the wavefunction.

The condition (37) has important consequences on the superconducting order. It is clear that in order to fulfill (37) $\Delta_{\mathbf{k}}$ must change sign in the Brillouin zone. In particular, since $w_1(\mathbf{k}) = -t_{\mathbf{k}}/(2\sqrt{2}t)$, $\Delta_{\mathbf{k}}$ is constant on surfaces of fixed energy:

$$\Delta_{\mathbf{k}} = \Delta(\xi_{\mathbf{k}}) = \Delta[1 + r(\xi_{\mathbf{k}} + \mu')/(2\sqrt{2}t)]. \tag{38}$$

Thus the line of nodes corresponds to a given energy $\xi_{\mathbf{k}}$ instead of given direction, as it would be in p- or d-wave superconductivity. The energy for which Δ vanishes is $\xi_N = -2\sqrt{2}t/r - \mu'$. Other consequences of (37) will be discussed in more details in Section IV D, after the solution of the self-consistent equations.

Before proceeding, we find a simpler expression for the relevant W's. Adding and subtracting μ' in the numerator of W_{10} we have:

$$W_{10} = -\frac{\mu'}{2\sqrt{2}t}W_{00} - \frac{1}{2\sqrt{2}t}\sum_{\mathbf{k}} \frac{\xi_{\mathbf{k}}}{2E_{\mathbf{k}}}.$$
 (39)

We use Eq. (24) fixing n to eliminate the second term. We obtain:

$$2\mu' W_{00} + 4\sqrt{2}tW_{10} = n - 1, \qquad (40)$$

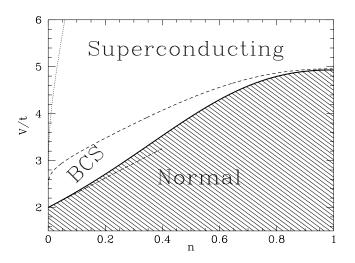


FIG. 2: Boundary between the s-wave superconductor and a normal phase. The dashed line is the line where $\Delta/(\mu'+D) = .1$, thus it gives an indication of the BCS region. The dotted line is the line where the chemical potential it exactly at the band edge: $\mu' = -D$, and can be considered the beginning of the Bose region. The dot-dashed line in the dashed region is the analytical expression of Eq. (46) valid for small n.

that is a generalization of Eq. (20) for the two-body problem. Similarly for W_{11} we have:

$$W_{11} = \frac{\mu'^2}{8t^2}W_{00} + \frac{\mu'(1-n)}{8t^2} + b \tag{41}$$

where

$$b = \frac{1}{16t^2} \sum_{\mathbf{k}} \frac{\xi_{\mathbf{k}}^2}{E_{\mathbf{k}}} = -\frac{\mu'}{16t^2} + \frac{1}{16t^2} \sum_{\mathbf{k}} \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} (\xi_{\mathbf{k}} - E_{\mathbf{k}})$$
 (42)

In conclusion we obtain the following set of equations:

$$\frac{1}{V} = 2b(\mu', \Delta, r) - \frac{(n-1)^2}{16t^2 W_{00}(\mu', \Delta, r)}$$
(43)

$$\frac{1}{r} = -\frac{\mu'}{2\sqrt{2}t} + \frac{n-1}{4\sqrt{2}tW_{00}(\mu', \Delta, r)}$$
(44)

This form is more convenient for the following discussion since b remains finite when $\Delta \to 0$.

Equations (43) and (44), together with Eq. (24), form the complete set of equations for the three unknowns $\{\mu', \Delta, r\}$ (the gap is defined in Eq. (35)). This will be our starting point to discuss the physics of the s-wave superconducting state.

A. Threshold line for s-wave superconductivity

We have seen that in the two-body problem a pair is bound only if V exceeds a threshold potential V_t^s . For small densities it is clear that for $V > V_t^s$ the system is

superconducting and in the Bose limit, i.e. with a coherence length much smaller that the average interparticle distance. As shown rigorously by Randeria et al. 17, in the low density limit and in 2D, the presence of a bound state in the two-body problem is a necessary and sufficient condition for s-wave superconducting instability to take place. We thus expect that for $V < V_t^s$ and $n \to 0$ the system is not superconducting. A separation line, starting at V_t^s for $n \to 0$, as function of n, separates the s-wave superconducting region and the normal behavior. The equation for this line of second-order transition can be found by setting $\Delta = 0$ in Eq. (43) n being fixed by the chemical potential μ' ($-4t < \mu' < 4t \equiv D$). We obtain:

$$\frac{1}{V} = -\frac{\mu'}{8t^2} + \frac{1}{8t^2} \sum_{\mathbf{k}} \left[|\xi_{\mathbf{k}}| - \xi_{\mathbf{k}} \right] . \tag{45}$$

When $\Delta = 0$, $\mu' + D = \epsilon_F^o$ is the Fermi energy of an ideal gas measured from the band edge. For small doping $\epsilon_F^o = 2\pi t n$, and since for small n the integral in (45) is quadratic in ϵ_F we can neglect it and find a simple analytic expression for the threshold curve:

$$\frac{V_t^s}{t} = 2 + \pi n + O(n^2). (46)$$

The complete curve is shown in Fig. 2. The critical line increases smoothly from V/t=2 for n=0 to $V/t\approx 4.93$ at half-filling (n=1). This can be easily understood by the fact that the particles feel more and more the presence of the hard-core repulsion.

B. Near the threshold: BCS limit

Near the transition line the system behaves like a BCS superconductor for weak coupling. In particular, the superconducting gap is much smaller than ϵ_F^o , the Fermi energy of the free gas, and μ' remains $-D + \epsilon_F^o$. In order to prove this fact we assume that these properties hold, and we evaluate Eq. (43). W_{00} has the usual $\ln \Delta$ divergent behavior and it can be evaluated in leading order by assuming a constant density of states and constant $\Delta_{\bf k}$ near the Fermi surface $(t_{\bf k} = \mu')$. It is convenient to write the equation in terms of $V - V_t^s(n)$, by subtracting the critical line equation. In this way we obtain:

$$\Delta(\mu') \approx 2\sqrt{D^2 - {\mu'}^2} \exp\left\{-\frac{(1-n)^2 V V_t(n)}{16t^2 [V - V_t(n)] \rho(\mu')}\right\},$$
(47)

where $\rho(\mu')$ is the density of states per spin evaluated at μ' . Near the threshold $\Delta/\epsilon_F^o \ll 1$ and thus the superconductor is of BCS type. Such a regime persists as long as $\Delta(\mu')/(\mu'+D)$ is small. The dashed line in Fig. 2 indicates the values of n and V for which $\Delta(\mu')/(\mu'+D)=0.1$. The "BCS region" is restricted between that line and the critical line V_t^s – a narrow region compared to the remainder of the phase diagram. The behavior of the chemical potential is shown in Fig. 4.

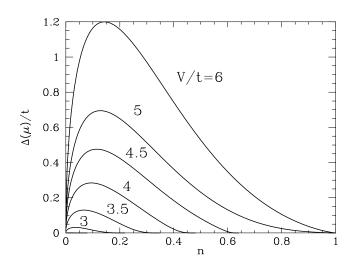


FIG. 3: Gap function at the Fermi energy $\Delta(\mu')/t$ as a function of the density n, and for different values of the coupling V. Starting with the upper curve V/t is: 6, 5, 4.5, 4, 3.5, 3, and 2.5. One can easily see the square-root behavior for small n, typical of a Bose behavior. For V < 4.93, near the critical point value of the density a BCS exponential decay is evident. For V > 4.93 and at half-filling, the gap function $\Delta(\mu')$ vanishes on the Fermi surface remaining finite elsewhere. Since at half-filling the model fails, we do not discuss further this behavior.

C. Bose limit and intermediate regime

As discussed above, for $V > V_t^s$ and small density we inevitably reach the Bose limit. This is confirmed by the mean field equations. Indeed for $n \to 0$ the quantity $\Delta/|\mu'+D|$ vanishes and $\mu'<-D$. One can thus verify that the Eq. (43) reduces to Eq. (22) for the bound state energy of the two-body problem with $\mu' = \omega_B/2$. At the same time Δ is fixed by Eq. (24) that gives $\Delta \sim t\sqrt{n}$. This behavior of Δ can be seen in Fig. 3 for small n. For intermediate couplings and densities the numerical solution crosses over between the BCS and Bose limits described above. In Fig. 5 we plot the lines of constant $\Delta(\mu')/(\mu'+D)$. We have seen that this ratio characterizes both the BCS (small positive value) and the Bose limit (small negative value). The phase diagram for the crossover from BCS to Bose condensation in the purely attractive case was given in Ref. 16 for both s-wave (local attraction) and d-wave (nearest neighbour attraction). A comparison of the results shows that the effect of the repulsion is to eliminate a large portion of the s-wave BCS region, which becomes normal. The d-wave case will be discussed in Section V.

All these curves are plotted in the range of densities (0,1): it should be stressed that the have no real meaning near half filling since the mean field approach misses the insulating state. We expect that the approximation remains valid as far as $z_k v$, the weight of the quasiparticle peak, remains of the order of 1. We also remember that

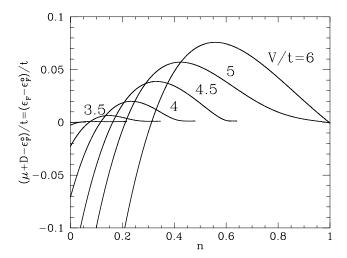


FIG. 4: The chemical potential μ' measured from the bottom of the band -D, minus the free gas Fermi energy ϵ_F^o . The curve are at fixed V/t which takes the values: 6, 5, 4.5, 4, 3.5, 3, and 2.5 from the top to the bottom curve. The comparison is particularly interesting near the critical value of n. There the behavior is BCS and the system is only slightly different from the free gas, since $\epsilon_F \approx \epsilon_F^o$ and $\Delta \ll \epsilon_F$. For V larger that 4.93 no critical density exists, and the system never become strictly BCS.

in the corresponding Kondo problem the limit n=1, corresponds to no particles at all.

D. Nodes of $\Delta(\xi)$

We have seen above that Δ depends only on ξ and that it vanishes for $\xi = \xi_N$. As a consequence we can write $\Delta(\xi)$ as follows:

$$\Delta(\xi) = \frac{\Delta r}{2\sqrt{2}t} [\xi - \xi_N] \tag{48}$$

where, substituting Eq. (44) in the expression for ξ_N we have:

$$\xi_N = \frac{1 - n}{2W_{00}(\mu', \Delta, r)}.$$
 (49)

For small value of Δ , $\xi_N \sim -t/\ln(\Delta/t)$, thus it vanishes logarithmically in Δ . This means that approaching the threshold line V_t^s the lines of nodes approach the Fermi surface. It turns out that keeping it at a logarithmically small distance (in Δ) suffices to fulfill the hard-core condition (37).

The presence of a line of nodes near the Fermi surface modifies the usual shape of the occupation number distribution $n_{\mathbf{k}}$. Specifically, it introduces a particle-hole asymmetry for $|\xi| \approx \xi_N$. For large values of the energy the n distribution is anomalous. Usually, far from the Fermi surface, $n_{\mathbf{k}}$ is either 0 or 1, depending on the sign

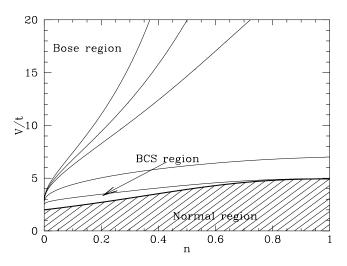


FIG. 5: Phase diagram of the model for n and V/t, $U=+\infty$. In the shaded region s-wave superconducting is not stable. In the rest of the diagram we find that s-wave superconductivity smoothly crosses from the BCS regime, near the critical line (the border of the shaded region), to the Bose regime, near the n=0 line. In order to characterize better this crossover we report the lines of fixed ratio $\Delta(\mu')/(\mu'+D)$. From the upper line to the critical line the ratio is ∞ , 10, 5, 1, and 1. Surprisingly the BCS region is narrow, and the genuine crossover region covers most of the diagram.

of ξ . In contrast our $\Delta(\xi)$ is $\sim \xi$ when $|\xi|$ is large with respect to both Δ and ξ_N , leading to

$$n(\xi) \approx \frac{1}{2} \left[1 - \text{sgn}(\xi) \frac{1}{\sqrt{1 + \Delta^2 r^2 / 8t^2}} \right] .$$
 (50)

This behavior can be recognized in Figure 6 where the form of $n(\xi)$ is shown for V/t = 4.5 and for two different values of n. Inspection of that figure shows that $n(\xi)$ remains symmetrical around the chemical potential only for $|\xi| \ll \Delta(\mu')$. The asymmetry for $|\xi| > \xi_N$ is clearly apparent in the inset.

The aforementioned asymmetry explains the anomalous behavior of the chemical potential in the superconducting state seen in Fig. 4. The chemical potential is normally shifted down with respect to the free gas value! The BCS distribution function is particle-hole symmetric, and states are "missing" below the lower band edge: μ must go down in order to retain the same density. In contrast here the lower spectral density near $\xi = \xi_N$ leads to an increase of μ in a narrow range where Δ and ξ_N are comparable, as shown in Figures 4 and 7.

V. d-WAVE SUPERCONDUCTIVITY

We consider now the possibility of d-wave superconductivity. By symmetry, the hard-core part of the interaction is not seen by the two-body wave function, thus the scattering states should always feel an attraction at

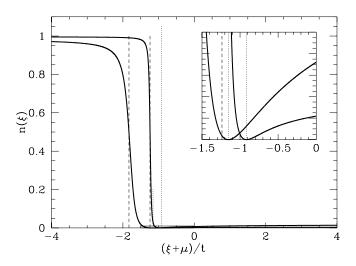


FIG. 6: Occupation number $n_{\mathbf{k}} = n(\xi_{\mathbf{k}})$ for V/t = 4.5 and two different values of n: n = 0.4 (left curve) and n = 0.642 (right curve). In the inset the region where $n_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ vanishes is shown enlarged. The dashed line indicates the value of the chemical potential, and the dotted one ξ_N .

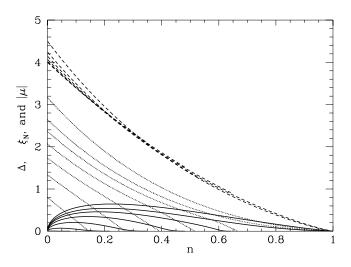


FIG. 7: The three relevant energy scales of the problem: (dashed lines) $|\mu|$, (dotted lines) ξ_N , and (full line) $\Delta(\mu)$ are plotted for the same values of V of Fig.3. As expected, ξ_N vanishes linearly in $n-n_t$, while Δ vanishes exponentially in $1/(n-n_t)$.

finite energy. This is enough to induce BCS superconductivity at any finite density and for any value of the coupling constant V. In contrast the Bose limit can be reached only if a bound state is present in the two body problem, $V > V_t^d = 7.35\,t$. Remember that in this limit s-wave always wins, we thus restrict to $V < V_t^d$.

In the opposite limit, for small values of the coupling $V \ll V_t^s$, the situation is again clear: we expect a standard BCS d-wave superconductors, since there is no s-wave solution there. (The presence of a small hopping at nearest neighbors is discussed in the next section and it

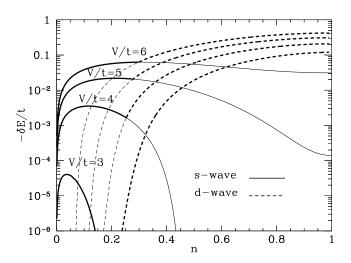


FIG. 8: Ground state energy gain $|\delta E|$ for s-(full lines) and d-wave (dashed lines) superconducting state as a function of the density for different values of V (indicated in the figure). The realized state is emphasized with a thicker line.

will not change the final outcome.)

The situation is much more interesting at intermediate couplings, $V_t^s < V < V_t^d$. In this region there is competition between the two possible superconducting orders: the lowest in energy will be the actual ground state. We analyze qualitatively this competition as a function of the density n for a fixed value of the coupling V. For small density $(n \to 0)$ the d-wave order parameter has a BCS-like form with an effective interaction $V_{eff} = V \langle w_2^2 \rangle_{FS}$ where $\langle w_2^2 \rangle_{FS}$ is the average over the Fermi surface of the angular factor. Since $w_2(\mathbf{k}) \sim (k_x^2 - k_y^2)$, V_{eff} , which is of order w_2^2 , is reduced by a factor n^2 . The gap $\Delta_{\mathbf{k}}$ is exponentially small and the resulting energy gain vanishes extremely rapidly with n since $\delta E \approx -\rho(\mu) \langle \Delta_{\mathbf{k}}^2 \rangle_{FS}/2$.

The s-wave solution, instead, is in the Bose limit, thus its energy gain is simply the number of bosons multiplied by the bound state energy: $\delta E = n\omega_B/2$. For $n \to 0$ the s-wave is always preferred to the d-wave.

The opposite holds near the threshold for s-superconductivity: there d-wave still lowers energy, and is thus preferred. We expect a first order transition in between. The question is "where"? Will the BCS s-region be completely sweeped out by the d-wave BCS state?

In order to answer this question we need an explicit calculation of the ground state energy gain for the superconducting state:

$$\delta E = 2\sum_{\mathbf{k}} t_{\mathbf{k}} n_{\mathbf{k}} - 2\sum_{\mathbf{k} < \mathbf{k}_F} t_{\mathbf{k}} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \mathcal{F}_{\mathbf{k}}.$$
 (51)

The last term in (51) is $-\Delta_d^2/(2V)$ for the d-wave symmetry, and $\Delta^2 r^2/(2V)$ for s-wave. Δ_d is obtained by solving Eq. (18) and Eq. (24) with $\Delta_{\mathbf{k}} = \Delta_d w_2(\mathbf{k})$. Δ and r are the quantities introduced in (35) and discussed in the previous Section. Numerical results are shown in

Fig. 8. One can clearly see the crossing of the two energy values indicating the first order transition. For small density, as expected, the s-wave state is always lower in energy (left side of the diagram). Note however that the value of the energy for which the transition takes place depends strongly on the value of V considered. We can distinguish two cases:

(i) V slightly above $V_t^s(n=0)$ the s-wave superconductivity spans the whole crossover from the Bose limit (for $n\to 0$) to the BCS one. The first order transition to the d-phase occurs deep in the s-BCS region. Note that this happens at tiny values of δE (for instance for $V=2.5\,t,\,\delta E_c/t<10^{-10}$). Between the s- and the d-wave superconducting phases there exists a region that for all practical purposes is normal. Increasing the density at fixed V one thus find that superconductivity is reentrant.

(ii) At larger values of V, the s- and d-state energies cross for a value of the energy gain reasonably large (of the same order of the maximum value achieved along the s-wave evolution). Thus a nearly monotonic behavior of δE results (cf. the line $V=6\,t$).

In conclusion we found that the d-wave competes with the s-wave only for large values of V. When V is near the threshold a quasi-normal region between the s-wave and the d-wave can survive, and the BCS-Bose crossover in s-wave can take place fully.

VI. NEXT NEIGHBOR HOPPING AND d-WAVE s-WAVE COMPETITION

In this Section we consider the effect of the inclusion of a nearest-neighbors hopping integral t'. The effect of this term on the superconducting critical temperature has been investigated in Ref.⁴ and in more details in Ref.⁵. Here we consider ground state properties and in agreement with Refs.^{4,5} we find that the introduction of t' strongly modifies the s-wave phase diagram. As a matter of fact, the threshold line V_t^s is washed out by an arbitrary small t'. A transparent proof of that has been given in Ref.⁵. We reproduce here their arguments for zero temperature. Equation (34) for Δ can be rewritten as follows:

$$\frac{1}{2VW_{00}} = \langle w_1^2 \rangle - \langle w_1 \rangle^2 = \langle (w_1 - \langle w_1 \rangle)^2 \rangle, \qquad (52)$$

where we have defined:

$$\langle g(\mathbf{k}) \rangle \equiv \sum_{\mathbf{k}} \frac{g(\mathbf{k})}{E_{\mathbf{k}}} / \sum_{\mathbf{k}} \frac{1}{E_{\mathbf{k}}}.$$
 (53)

When Δ is small, the weighted average over the Brillouin zone is peaked on the Fermi surface. If $w_1(\mathbf{k})$ has the same \mathbf{k} dependence of the kinetic energy, the right-hand side of (52) vanishes at leading order in Δ , and the logarithmic divergence in W_{00} will be ineffective: superconductivity exists for V larger than a threshold V_t . In

contrast, when the spectrum $t_{\mathbf{k}}$ is such that $w_1(\mathbf{k})$ varies on the Fermi surface, the right-hand side of (52) is finite for $\Delta \to 0$ and superconductivity is possible however small V.

This is discussed extensively in⁵. Here we want to point out two interrelated facts: (i) the relation of superconductivity with the presence of a bound state in the two-body problem. (ii) The unusual nature of the superconducting state created by a small t' in the region of the phase diagram where the system would be normal but for t'.

Randeria et al.¹⁷ proved, within a two-dimensional continuum model, that the existence of an s-wave bound state for the two-body problem is a necessary and sufficient condition for the existence of s-wave superconductivity at low density. In the model at hand the presence of a small $t' \neq 0$ makes superconductivity always possible while it maintains a threshold for the two-body bound state. That threshold stems from the fact that w_1 has no fluctuations near the band edge – hence no $\log \omega_B$ term in the pair propagator. This result seems to contradict the prediction of Ref.¹⁷.

The solution of this inconsistency comes from the ${\bf k}$ dependence of Δ at the Fermi surface. In fact, even if the order parameter is of s-wave symmetry, it actually changes sign 8 times on the Fermi surface and it has a zero average on it. This can be verified by solving the set of Eqs. (31) and (24) in power series of t'. One finds the following expression for $\Delta_{\bf k}$:

$$\Delta_{\mathbf{k}} = \Delta \frac{t'}{\mu'} \left[v(\mathbf{k}) - \langle v \rangle_{FS} \right] + O(t'^2/\mu')$$
 (54)

where $t_{\mathbf{k}} = -2t\sqrt{2} w_1(\mathbf{k}) + t'v(\mathbf{k})$. More generally, it is clear that for any perturbation $v(\mathbf{k})$ to the nearest neighbor hopping, $\Delta_{\mathbf{k}}$ will change sign on the Fermi surface, and since it has s-wave symmetry this must happen at least 8 times.

Due to the unusual behavior of $\Delta_{\mathbf{k}}$ the results of Randeria *et al.* do not apply to this s-wave state which is, in practice, close to an angular momentum l=4 state (which is isotropic as regards cubic symmetry.)

Hence s-wave superconductivity survives the hard core for arbitrary small values of the attraction. But since the superconducting state is close to l=4, the resulting value of Δ (or T_c) is extremely small, even compared to the d-wave solution. We checked explicitly this fact for our model. We considered values of t' < t/2, since at this value the Fermi surface becomes double sheeted. We calculated the effective s-wave coupling

$$V_{eff}^{s}/V = \langle w_1^2 \rangle - \langle w_1 \rangle^2 \sim \left[\langle v^2 \rangle - \langle v \rangle^2 \right] t'^2 / (8t^2) \quad (55)$$

as a function of the Fermi energy and of the coupling t'. We compared V^s_{eff} with the effective d-wave coupling: $V^d_{eff}/V = \langle w^2_2 \rangle$. In all cases we found that $V^d_{eff} > V^s_{eff}$.

We thus conclude that the introduction of a $t^\prime < t/2$, or of other similar perturbations, does not change qualitatively the above discussion, since d-wave superconductivity always hides this anomalous s-wave state.

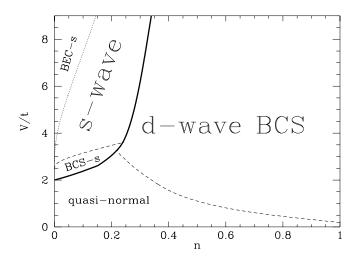


FIG. 9: Phase diagram considering the competition between s- and d-wave. The thick line corresponds to the first-order phase transition between the s- and d-wave superconducting order. On the s-side we indicate the BCS and Bose condensation regions. On the d-side the region where $\delta E/t < 10^{-6}$ is labeled as "quasi-normal".

VII. CONCLUSIONS

We have studied the appearance of superconductivity on a 2D lattice in presence of a hard-core repulsion and of a nearest neighbor attraction. We constructed the mean field solution and compared it to the two-body problem in vacuum. Even if the procedure is restricted to mean field, it correctly forbids the double occupancy of the same site of the superconducting wavefunction. The main results are the following: (i) the s-wave solution is suppressed

for small values of the coupling at any density. The introduction of additional small hopping integrals cannot change this, since the d-wave solution is always preferred. (ii) the d-wave solution is always possible, but the actual value of the energy gain becomes extremely small at low density. Thus for small V and n the critical temperatures are tiny: in practice at any temperature the system is normal. (iii) For V larger than the threshold for the s two body-bound state the system exhibits a crossover from the Bose-Einstein condensation of fermions pairs to a BCS behavior as the density is increased. A first order transition to the d-wave state occurs. The situation is summarized in the phase diagram of Fig. 9.

When only nearest neighbor attraction is present the competition between d-wave and s-wave at T_c has been considered recently by Wallington and Annett¹⁹. They found that for any coupling the s-wave has the lowest critical temperature, but for a small region near half-filling, where the van Hove singularity of density of states weighted with the angular factors stabilizes the d-wave phase. The presence of the hard-core repulsion allows d-wave superconductivity to appear on a much larger portion of the phase diagram. The correct treatment of the repulsion is thus crucial to study the competition between s- and d-wave.

The technical procedure developed can be applied to the Kondo-lattice problem sketched in the introduction. However, one has to keep in mind that in that problem superconductivity and Kondo hybridization should be considered on the same footing, since each of the two order parameter reacts on the other. We will not try thus to apply the above result *directly* to the Kondo lattice model: we leave the detailed solution of the superconductivity-Kondo hybridization in presence of the hard-core repulsion for future work²⁰.

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